Krzysztof B BeÄ

List of Publications by Year
in descending order

82	2,177	218381	253896
papers	citations	26 h-index	43 g-index

88	88	88	1045
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rapid discrimination of Curcuma longa and Curcuma xanthorrhiza using Direct Analysis in Real Time Mass Spectrometry and Near Infrared Spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 265, 120347.	2.0	14
2	Quantification of Silymarin in Silybi mariani fructus: Challenging the Analytical Performance of Benchtop vs. Handheld NIR Spectrometers on Whole Seeds. Planta Medica, 2022, 88, 20-32.	0.7	6
3	Physical principles of infrared spectroscopy. Comprehensive Analytical Chemistry, 2022, , 1-43.	0.7	9
4	Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. Foods, 2022, 11, 1465.	1.9	64
5	In silico NIR spectroscopy â€“ A review. Molecular fingerprint, interpretation of calibration models, understanding of matrix effects and instrumental difference. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 279, 121438.	2.0	13
6	Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines. , 2022, , 603-627.		1
7	Theae nigrae folium: Comparing the analytical performance of benchtop and handheld near-infrared spectrometers. Talanta, 2021, 221, 121165.	2.9	39
8	Near-infrared spectroscopy in quality control of Piper nigrum: A comparison of performance of benchtop and handheld spectrometers. Talanta, 2021, 223, 121809.	2.9	36
9	Issues in Hyperspectral Traceability of Foods. , 2021, , 258-289.		2
10	Challenging handheld NIR spectrometers with moisture analysis in plant matrices: Performance of PLSR vs. GPR vs. ANN modelling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119342.	2.0	29
11	NIR spectroscopy of natural medicines supported by novel instrumentation and methods for data analysis and interpretation. Journal of Pharmaceutical and Biomedical Analysis, 2021, 193, 113686.	1.4	43
12	Principles and Applications of Miniaturized Nearâ€Infrared (NIR) Spectrometers. Chemistry - A European Journal, 2021, 27, 1514-1532.	1.7	169
13	Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase. Chemical Society Reviews, 2021, 50, 10917-10954.	18.7	34
14	The comprehensive sourcebook for modern NIR spectroscopy: A commentary on â€œNear-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applicationsâ€• NIR News, 2021, 32, 5-10.	1.6	1
15	Novel near-infrared and Raman spectroscopic technologies for print and photography identification, classification, and authentication. NIR News, 2021, 32, 11-16.	1.6	2
16	ATR-far-ultraviolet spectroscopy in the condensed phaseâ€”The present status and future perspectives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 253, 119549.	2.0	14
17	Current and future research directions in computer-aided near-infrared spectroscopy: A perspective. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119625.	2.0	26
18	Theoretical Simulation of Near-Infrared Spectrum of Piperine: Insight into Band Origins and the Features of Regression Models. Applied Spectroscopy, 2021, 75, 1022-1032.	1.2	20

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19	Anharmonic DFT Study of Near-Infrared Spectra of Caffeine: Vibrational Analysis of the Second Overtones and Ternary Combinations. Molecules, 2021, 26, 5212.	1.7	12
20	Spectra-structure correlations in NIR region of polymers from quantum chemical calculations. The cases of aromatic ring, C=O, Câ‰¡N and C-Cl functionalities. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 262, 120085.	2.0	26
21	Insect Protein Content Analysis in Handcrafted Fitness Bars by NIR Spectroscopy. Gaussian Process Regression and Data Fusion for Performance Enhancement of Miniaturized Cost-Effective Consumer-Grade Sensors. Molecules, 2021, 26, 6390.	1.7	25
22	A Simple guide to complex world of overtone and combination bands: Theoretical simulation and interpretation of NIR spectra â€“ summary of the workshop at NIR-2021 Beijing Conference. NIR News, 2021, 32, 15-18.	1.6	2
23	Anharmonicity and Spectraâ€“Structure Correlations in MIR and NIR Spectra of Crystalline Menadione (Vitamin K3). Molecules, 2021, 26, 6779.	1.7	5
24	Near-Infrared (NIR) Sensors in Environmental Analysis. , 2021, , .		2
25	Scald-Cold: Joint Austrian-Italian consortium in the Euregio project for the comprehensive dissection of the superficial scald in apples. NIR News, 2020, 31, 5-9.	1.6	1
26	Principles and Applications of Vibrational Spectroscopic Imaging in Plant Science: A Review. Frontiers in Plant Science, 2020, 11, 1226.	1.7	35
27	Near-Infrared Spectroscopy as a Rapid Screening Method for the Determination of Total Anthocyanin Content in Sambucus Fructus. Sensors, 2020, 20, 4983.	2.1	29
28	Effect of conformational isomerism on NIR spectra of ethanol isotopologues. Spectroscopic and anharmonic DFT study. Journal of Molecular Liquids, 2020, 310, 113271.	2.3	14
29	Vibrational coupling to hydration shell â€“ Mechanism to performance enhancement of qualitative analysis in NIR spectroscopy of carbohydrates in aqueous environment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 237, 118359.	2.0	17
30	Near-Infrared Spectroscopy in Bio-Applications. Molecules, 2020, 25, 2948.	1.7	185
31	Biomolecular and bioanalytical applications of infrared spectroscopy â€“ A review. Analytica Chimica Acta, 2020, 1133, 150-177.	2.6	107
32	Handheld near-infrared spectrometers: Where are we heading?. NIR News, 2020, 31, 28-35.	1.6	96
33	Comparative studies of vibrational properties and phase transitions in perovskiteâ€like frameworks of [(C 3 H 7) 4 N][M(N(CN) 2) 3] with Mï¿¾Mn, Co, Ni. Journal of Raman Spectroscopy, 2019, 50, 1561-1571.	1.2	6
34	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. Journal of Physical Chemistry B, 2019, 123, 10001-10013.	1.2	18
35	The essential role of omni-capable research laboratories in advancing analytical spectroscopy. NIR News, 2019, 30, 30-34.	1.6	0
36	Spectraâ€“Structure Correlations in Isotopomers of Ethanol (CX3CX2OX; X = H, D): Combined Near-Infrared and Anharmonic Computational Study. Molecules, 2019, 24, 2189.	1.7	19

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37	Overtones of Î½Câ‰¡N Vibration as a Probe of Structure of Liquid CH₃CN, CD₃CN, and CCl₃CN: Combined Infrared, Near-Infrared, and Raman Spectroscopic Studies with Anharmonic Density Functional Theory Calculations. Journal of Physical Chemistry A, 2019, 123, 4431-4442.	1.1	27
38	Recent advances in modeling vibrational spectra of food adulterants â€“ Theoretical simulation of IR and NIR bands of melamine. NIR News, 2019, 30, 5-10.	1.6	2
39	The fundamental handbook for analytical spectroscopy. Release of the second edition of â€˜Chemometrics in spectroscopyâ€™ by Howard Mark and Jerry Workman, Jr. and its impact on the spectroscopic community. NIR News, 2019, 30, 11-13.	1.6	0
40	Distinct Difference in Sensitivity of NIR vs. IR Bands of Melamine to Inter-Molecular Interactions with Impact on Analytical Spectroscopy Explained by Anharmonic Quantum Mechanical Study. Molecules, 2019, 24, 1402.	1.7	38
41	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. Scientific Reports, 2019, 9, 17398.	1.6	20
42	Advances in Near-Infrared Spectroscopy and Related Computational Methods. Molecules, 2019, 24, 4370.	1.7	13
43	The use of vibrational spectroscopy in medicinal plant analysis: current and future directions. Planta Medica, 2019, 85, .	0.7	2
44	Breakthrough Potential in Near-Infrared Spectroscopy: Spectra Simulation. A Review of Recent Developments. Frontiers in Chemistry, 2019, 7, 48.	1.8	170
45	NIR spectroscopy in simulation â€“ a new way for augmenting near-infrared phytoanalysis. , 2019, 85, .		0
46	Quantum mechanical modeling of NIR spectra of thymol. , 2019, 85, .		0
47	Handling of uncertainty due to interference fringe in FT-NIR transmittance spectroscopy â€” Performance comparison of interference elimination techniques using glucose-water system. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 208-215.	2.0	7
48	Spectra-structure correlations in NIR region: Spectroscopic and anharmonic DFT study of n-hexanol, cyclohexanol and phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 176-184.	2.0	33
49	Rydberg transitions as a probe for structural changes and phase transition at polymer surfaces: an ATR-FUV-DUV and quantum chemical study of poly(3-hydroxybutyrate) and its nanocomposite with graphene. Physical Chemistry Chemical Physics, 2018, 20, 8859-8873.	1.3	20
50	Advances in Anharmonic Methods and Their Applications to Vibrational Spectroscopies. , 2018, , 483-512.		9
51	Electronic Spectra of Graphene in Far- and Deep-Ultraviolet Region: Attenuated Total Reflection Spectroscopy and Quantum Chemical Calculation Study. Journal of Physical Chemistry C, 2018, 122, 28998-29008.	1.5	9
52	Computer simulations of NIR spectra of thymol â€“ Towards linking basic and analytical NIRS. NIR News, 2018, 29, 13-16.	1.6	3
53	Near-IR Spectroscopy and Its Applications. , 2018, , 11-38.		24
54	Quantum mechanical simulations of near-infrared spectra of biomolecules â€“ Long-chain fatty acids. NIR News, 2018, 29, 13-19.	1.6	3

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55	NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features. Journal of Molecular Liquids, 2018, 268, 895-902.	2.3	42
56	NIR Spectra Simulations by Anharmonic DFT-Saturated and Unsaturated Long-Chain Fatty Acids. Journal of Physical Chemistry B, 2018, 122, 6931-6944.	1.2	39
57	Influence of Non-fundamental Modes on Mid-infrared Spectra: Anharmonic DFT Study of Aliphatic Ethers. Journal of Physical Chemistry A, 2017, 121, 1412-1424.	1.1	27
58	Correlations between Structure and Near-Infrared Spectra of Saturated and Unsaturated Carboxylic Acids. Insight from Anharmonic Density Functional Theory Calculations. Journal of Physical Chemistry A, 2017, 121, 3437-3451.	1.1	64
59	Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids. Near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 35-44.	2.0	38
60	Critical Evaluation of NIR and ATR-IR Spectroscopic Quantifications of Rosmarinic Acid in Rosmarini folium Supported by Quantum Chemical Calculations. Planta Medica, 2017, 83, 1076-1084.	0.7	25
61	Temperature Drift of Conformational Equilibria of Butyl Alcohols Studied by Near-Infrared Spectroscopy and Fully Anharmonic DFT. Journal of Physical Chemistry A, 2017, 121, 1950-1961.	1.1	48
62	Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in Rosmarini folium. Analyst, The, 2017, 142, 455-464.	1.7	94
63	Spectroscopic and Quantum Mechanical Calculation Study of the Effect of Isotopic Substitution on NIR Spectra of Methanol. Journal of Physical Chemistry A, 2017, 121, 7925-7936.	1.1	29
64	Interpretation of the Ãƒ â†•Xì‚ transition of hydrated protons in aqueous solutions observed in the far-UV region with quantum chemical calculations. Physical Chemistry Chemical Physics, 2017, 19, 21490-21499.	1.3	6
65	Quantum chemical calculation of NIR spectra of practical materials. NIR News, 2017, 28, 13-20.	1.6	12
66	FUV-DUV spectra of graphene, carbon nanotubes, and polymer nanocomposites (Conference) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 302	0	
67	Quantum Chemical Calculations of Basic Molecules: Alcohols and Carboxylic Acids. NIR News, 2016, 27, 15-21.	1.6	14
68	A spectroscopic and theoretical study in the near-infrared region of low concentration aliphatic alcohols. Physical Chemistry Chemical Physics, 2016, 18, 13666-13682.	1.3	72
69	Spectroscopic and Computational Study of Acetic Acid and Its Cyclic Dimer in the Near-Infrared Region. Journal of Physical Chemistry A, 2016, 120, 6170-6183.	1.1	44
70	Computational and quantum chemical study on high-frequency dielectric function of tert-butylmethyl ether in mid-infrared and near-infrared regions. Journal of Molecular Liquids, 2016, 224, 1189-1198.	2.3	9
71	On optimization of absorptionâ€“dispersion spectra. Journal of Molecular Structure, 2016, 1126, 11-18.	1.8	1
72	Dielectric functions of iso -propanol and di- iso -propylether in the infrared. Journal of Molecular Liquids, 2015, 203, 143-152.	2.3	3

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73	Vibrational analysis of neat liquid tert-butylmethylether. Journal of Molecular Liquids, 2014, 196, 26-31.	2.3	14
74	Vibrational analysis of liquid n-butylmethylether. Vibrational Spectroscopy, 2013, 64, 164-171.	1.2	13
75	Infrared dispersion of liquid di-n-propylether. Journal of Molecular Liquids, 2013, 181, 127-132.	2.3	6
76	Infrared Optical Constants and Computational Studies of Neat Liquid -Butylethylether. Journal of Spectroscopy, 2013, 2013, 1-8.	0.6	3
77	Analysis of Infrared Spectra of Neat Liquid N-Methylpyrrole. Acta Physica Polonica A, 2013, 124, 115-121.	0.2	6
78	Optical constants of liquid pyrrole in the infrared. Journal of Molecular Liquids, 2012, 172, 34-40.	2.3	18
79	Thin film IR and computational studies of liquid di-n-butylether. Journal of Molecular Structure, 2012, 1026, 51-58.	1.8	4
80	Vibrational spectra of liquid di-iso-propylether. Vibrational Spectroscopy, 2011, 55, 44-48.	1.2	10
81	Vibrational spectra of liquid di-n-propylether. Journal of Molecular Structure, 2010, 975, 205-210.	1.8	8
82	SciX 2021 summary including NIR spectroscopy session. NIR News, 0, , 096033602210763.	1.6	0